

A stability analysis of a real space split operator method for the Klein-Gordon equation

Frederick Blumenthal and Heiko Bauke*

Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany

We carry out a stability analysis for the real space split operator method for the propagation of the time-dependent Klein-Gordon equation that has been proposed Ruf et al. [M. Ruf, H. Bauke, C.H. Keitel, A real space split operator method for the Klein-Gordon equation, *Journal of Computational Physics* 228 (24) (2009) 9092–9106, doi:10.1016/j.jcp.2009.09.012]. The region of algebraic stability is determined analytically by means of a von-Neumann stability analysis for systems with homogeneous scalar and vector potentials. Algebraic stability implies convergence of the real space split operator method for smooth absolutely integrable initial conditions. In the limit of small spatial grid spacings h in each of the d spatial dimensions and small temporal steps τ , the stability condition becomes $h/\tau > \sqrt{d}c$ for second order finite differences and $\sqrt{3}h/(2\tau) > \sqrt{d}c$ for fourth order finite differences, respectively, with c denoting the speed of light. Furthermore, we demonstrate numerically that the stability region for systems with inhomogeneous potentials coincides almost with the region of algebraic stability for homogeneous potentials.

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1. Introduction

The Klein-Gordon equation is a partial differential equation that governs the quantum evolution of wave functions for relativistic spinless particles. It finds its applications for example in modeling light matter interaction in the relativistic regime [1–3]. The derivation of analytical solutions for the time-dependent problems in relativistic quantum dynamics requires sophisticated mathematical tools [4–9] and many setups necessitate numerical approaches solving the Dirac equation [10–17] or the Klein-Gordon equation [16, 18], especially problems with time-dependent potentials. In weakly relativistic regimes the solution of the Pauli equation with first order relativistic corrections may be sufficient [19].

Ruf et al. [20] developed an explicit real space split operator finite difference scheme for the numerical solution of the time-dependent Klein-Gordon equation. It has been applied for example to study relativistic ionization characteristics of laser-driven hydrogen like ions [16] and numerical signatures of non-self-adjointness in quantum Hamiltonians [21]. As an explicit scheme, the real space split operator finite difference scheme allows for an efficient implementation on distributed memory parallel computers. Explicit finite difference schemes for hyperbolic partial differential equations, however, are known to be never unconditionally stable [22, 23]. This means, that the numerical error that is caused by the application of an explicit finite difference scheme to the Klein-Gordon equation will grow exponentially unless the spatial and temporal grid spacings fulfill certain conditions. The purpose of this contribution is to study the stability of the explicit real space split operator finite difference scheme as introduced in [20] and to derive stability conditions for this scheme.

The reminder of the paper is organized as follows. In order to keep the paper self-contained, we will give a brief description of the real space split operator method for the Klein-Gordon equation in Sec. 2. Section 3 will state more precisely the notion of numerical stability by defining strong and algebraic stability, while Sec. 4 reviews conditions for these notions of stability. A von-Neumann stability analysis for constant potentials will be performed in Sec. 5 and in Sec. 6 we will compare our theoretical results with the stability of an actual computer implementation of the real space split operator method for systems with homogeneous potentials as well as for systems with spatial dependent potentials.

2. A real space split operator method for the Klein-Gordon equation

The Klein-Gordon equation—sometimes also called Klein-Fock-Gordon or Klein-Gordon-Schrödinger equation—is an equation of motion for a complex-valued scalar quantum wave function $\varphi(x, t)$ [8, 24, 25]. It governs the behavior of a charged spinless

* heiko.bauke@mpi-hd.mpg.de

particle with mass m and charge q moving under the effect of electrodynamic potentials $\mathbf{A}(\mathbf{x}, t)$ and $\phi(\mathbf{x}, t)$. Introducing the speed of light c and the reduced Planck constant \hbar , the scalar Klein-Gordon equation reads

$$\left[\left(i\hbar \frac{\partial}{\partial t} - q\phi(\mathbf{x}, t) \right)^2 - c^2 (-i\hbar \nabla - q\mathbf{A}(\mathbf{x}, t))^2 - m^2 c^4 \right] \varphi(\mathbf{x}, t) = 0. \quad (1)$$

This hyperbolic partial differential equation is of second order in time. For numerical purposes a transformation of (1) into a first order partial differential equation is advantageous. Introducing the two-component wave function [24]

$$\Psi(\mathbf{x}, t) = \begin{pmatrix} \Psi_1(\mathbf{x}, t) \\ \Psi_2(\mathbf{x}, t) \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \left(\varphi(\mathbf{x}, t) + \frac{1}{mc^2} \left(i\hbar \frac{\partial}{\partial t} - q\phi(\mathbf{x}, t) \right) \varphi(\mathbf{x}, t) \right) \\ \frac{1}{2} \left(\varphi(\mathbf{x}, t) - \frac{1}{mc^2} \left(i\hbar \frac{\partial}{\partial t} - q\phi(\mathbf{x}, t) \right) \varphi(\mathbf{x}, t) \right) \end{pmatrix} \quad (2)$$

the Klein-Gordon equation (1) may be transformed into Schrödinger form with the Hamiltonian operator \hat{H} , viz.

$$i\hbar \frac{\partial \Psi(\mathbf{x}, t)}{\partial t} = \hat{H}(t) \Psi(\mathbf{x}, t) = \left(\frac{\sigma_3 + i\sigma_2}{2m} (-i\hbar \nabla - q\mathbf{A}(\mathbf{x}, t))^2 + q\phi(\mathbf{x}, t) + \sigma_3 mc^2 \right) \Psi(\mathbf{x}, t). \quad (3)$$

The wave-function's components are related by the complex Hermitian unitary Pauli matrices σ_2 and σ_3 that obey the Pauli algebra

$$\sigma_i \sigma_j = i\epsilon_{i,j,k} \sigma_k + \delta_{i,j}, \quad (4a)$$

$$[\sigma_i, \sigma_j] = 2i\epsilon_{i,j,k} \sigma_k, \quad (4b)$$

$$\{\sigma_i, \sigma_j\} = 2\delta_{i,j}, \quad (4c)$$

with $i, j, k \in \{1, 2, 3\}$ and where $\epsilon_{i,j,k}$ denotes the permutation symbol and $\delta_{i,j}$ is the Kronecker delta. The Pauli algebra does not define the Pauli matrices uniquely. In numerical applications, we choose the representation

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (5)$$

Solutions $\Psi(\mathbf{x}, t)$ of equation (3) satisfy the continuity equation

$$\frac{\partial \rho(\mathbf{x}, t)}{\partial t} + \nabla \cdot \mathbf{j}(\mathbf{x}, t) = 0 \quad (6)$$

with the density

$$\rho(\mathbf{x}, t) = \Psi^*(\mathbf{x}, t) \sigma_3 \Psi(\mathbf{x}, t) = |\Psi_1(\mathbf{x}, t)|^2 - |\Psi_2(\mathbf{x}, t)|^2. \quad (7)$$

and the current

$$\mathbf{j}(\mathbf{x}, t) = -\frac{i\hbar}{2m} [\Psi^*(\mathbf{x}, t) \sigma_3 (\sigma_3 + i\sigma_2) \nabla \Psi(\mathbf{x}, t) - (\nabla \Psi^*(\mathbf{x}, t)) \sigma_3 (\sigma_3 + i\sigma_2) \Psi(\mathbf{x}, t)] - \frac{q\mathbf{A}(\mathbf{x}, t)}{m} \Psi^*(\mathbf{x}, t) \sigma_3 (\sigma_3 + i\sigma_2) \Psi(\mathbf{x}, t), \quad (8)$$

where $\Psi^*(\mathbf{x}, t)$ denotes the complex conjugate of $\Psi(\mathbf{x}, t)$. The density (7) is not positive definite and, therefore, the integral

$$\|\Psi(\mathbf{x}, t)\|_{\sigma_3}^2 = \int \Psi^*(\mathbf{x}, t) \sigma_3 \Psi(\mathbf{x}, t) d\mathbf{x}^d \quad (9)$$

over the d -dimensional space is not a norm and $\rho(\mathbf{x}, t)$ cannot be interpreted as a probability density and $\mathbf{j}(\mathbf{x}, t)$ is not a probability density current. The quantity $q\rho(\mathbf{x}, t)$, however, may be interpreted as a charge density and $q\mathbf{j}(\mathbf{x}, t)$ as a charge current [5–8, 24]. The conservation of the pseudo norm (9) implies charge conservation. Note that the Euclidean norm

$$\|\Psi(\mathbf{x}, t)\|^2 = \int \Psi^*(\mathbf{x}, t) \Psi(\mathbf{x}, t) d\mathbf{x}^d \quad (10)$$

is not conserved under the evolution of the Klein-Gordon equation.

In order to derive the real space split operator method of [20], we start from the formal solution of (3) with the initial condition $\Psi(\mathbf{x}, 0)$ that may be expressed as

$$\Psi(\mathbf{x}, t) = \hat{U}(t, 0) \Psi(\mathbf{x}, 0) \quad (11)$$

by introducing the unitary time-evolution operator [26]

$$\hat{U}(t_2, t_1) = \hat{T} \exp \left(-\frac{i}{\hbar} \int_{t_1}^{t_2} \hat{H}(t') dt' \right), \quad (12)$$

and Dyson's time ordering operator \hat{T} . The time-evolution operator $\hat{U}(t_2, t_1)$ effects the wave-function's evolution from time t_1 to time t_2 . Let $\hat{O}(t)$ denote some possibly time-dependent operator and define the operator

$$\hat{U}_{\hat{O}}(t_2, t_1, \delta) = \exp \left(-\delta \frac{i}{\hbar} \int_{t_1}^{t_2} \hat{O}(t') dt' \right), \quad (13)$$

that depends on the times t_1 and t_2 and the auxiliary parameter δ . Expanding $\hat{U}(t + \tau, t)$ to the third order in τ and introducing the operators

$$\hat{K}(\mathbf{x}, t) = \frac{\sigma_3 + i\sigma_2}{2m} (-i\hbar\nabla - q\mathbf{A}(\mathbf{x}, t))^2 \quad (14a)$$

$$\hat{V}(\mathbf{x}, t) = q\phi(\mathbf{x}, t) + \sigma_3 mc^2, \quad (14b)$$

the time-evolution operator for the Klein-Gordon equation (12) can be factorized as

$$\begin{aligned} \hat{U}(t + \tau, t) &= \exp \left(-\frac{i}{\hbar} \int_t^{t+\tau} \hat{H}(t') dt' \right) + O(\tau^3) \\ &= \hat{U}_{\hat{V}} \left(t + \tau, t, \frac{1}{2} \right) \hat{U}_{\hat{K}}(t + \tau, t, 1) \hat{U}_{\hat{V}} \left(t + \tau, t, \frac{1}{2} \right) + O(\tau^3). \end{aligned} \quad (15)$$

Neglecting terms of order $O(\tau^3)$, equation (15) gives an explicit second order accurate time-stepping scheme for the propagation of the Klein-Gordon wave function $\Psi(\mathbf{x}, t)$.

The operator $\hat{U}_{\hat{V}}(t + \tau, t, \delta)$ is diagonal in real space and explicitly given by

$$\hat{U}_{\hat{V}}(t + \tau, t, \delta) \Psi(\mathbf{x}, t) = \begin{pmatrix} \exp \left(-\delta \frac{i}{\hbar} \int_t^{t+\tau} q\phi(\mathbf{x}, t') + mc^2 dt' \right) \Psi_1(\mathbf{x}, t) \\ \exp \left(-\delta \frac{i}{\hbar} \int_t^{t+\tau} q\phi(\mathbf{x}, t') - mc^2 dt' \right) \Psi_2(\mathbf{x}, t) \end{pmatrix}. \quad (16)$$

The action of the operator $\hat{U}_{\hat{K}}(t + \tau, t, \delta)$ on $\Psi(\mathbf{x}, t)$ may be calculated by the Taylor series of the exponential function

$$\begin{aligned} \hat{U}_{\hat{K}}(t + \tau, t, \delta) \Psi(\mathbf{x}, t) &= \exp \left(-\delta \frac{i}{\hbar} \int_t^{t+\tau} \hat{K}(\mathbf{x}, t') dt' \right) \Psi(\mathbf{x}, t) \\ &= \sum_{j=0}^{\infty} \frac{1}{j!} \left[-\delta \frac{i}{\hbar} \int_t^{t+\tau} \frac{\sigma_3 + i\sigma_2}{2m} \left(\frac{\hbar}{i} \nabla - q\mathbf{A}(\mathbf{x}, t') \right)^2 dt' \right]^j \Psi(\mathbf{x}, t). \end{aligned} \quad (17)$$

Recognizing that all but the first two terms of the infinite series (17) vanish because the operator $(\sigma_3 + i\sigma_2)$ is nilpotent, that is, $(\sigma_3 + i\sigma_2)^2 = 0$, yields

$$\hat{U}_{\hat{K}}(t + \tau, t, \delta) \Psi(\mathbf{x}, t) = \Psi(\mathbf{x}, t) - (\sigma_3 + i\sigma_2) \frac{\delta i}{2m\hbar} \int_t^{t+\tau} \left(\frac{\hbar}{i} \nabla - q\mathbf{A}(\mathbf{x}, t') \right)^2 \Psi(\mathbf{x}, t) dt'. \quad (18)$$

Introducing the quantities

$$c_0 = \exp \left(-\frac{qi}{2\hbar} \int_t^{t+\tau} \phi(\mathbf{x}, t') dt' \right), \quad (19a)$$

$$c_1 = \frac{i\tau\hbar}{2m}, \quad (19b)$$

$$c_2 = \frac{q}{m} \int_t^{t+\tau} \mathbf{A}(\mathbf{x}, t') dt', \quad (19c)$$

$$c_3 = \int_t^{t+\tau} \frac{q}{2m} \nabla \cdot \mathbf{A}(\mathbf{x}, t') - \frac{iq^2}{2m\hbar} \mathbf{A}(\mathbf{x}, t')^2 dt', \quad (19d)$$

and taking advantage of the standard representation (5) of the Pauli matrices the operator product (15) finally may be transformed into a product of the compact matrices

$$\hat{U}(t + \tau, t) = \overbrace{\begin{pmatrix} c_0 & 0 \\ 0 & c_0 \end{pmatrix}}^{(*)} \begin{pmatrix} e^{-imc^2\tau/(2\hbar)} & 0 \\ 0 & e^{+imc^2\tau/(2\hbar)} \end{pmatrix} \begin{pmatrix} 1 + (c_1 \nabla^2 + \mathbf{c}_2 \cdot \nabla + c_3) & (c_1 \nabla^2 + \mathbf{c}_2 \cdot \nabla + c_3) \\ -(c_1 \nabla^2 + \mathbf{c}_2 \cdot \nabla + c_3) & 1 - (c_1 \nabla^2 + \mathbf{c}_2 \cdot \nabla + c_3) \end{pmatrix} \begin{pmatrix} c_0 & 0 \\ 0 & c_0 \end{pmatrix} \begin{pmatrix} e^{-imc^2\tau/(2\hbar)} & 0 \\ 0 & e^{+imc^2\tau/(2\hbar)} \end{pmatrix} + O(\tau^3). \quad (20)$$

In a computer implementation of the real space split operator method, the wave function $\Psi(\mathbf{x}, t)$ is discretized on a rectangular $(d + 1)$ -dimensional space-time lattice with spatial grid spacings h_i ($i \in \{1, \dots, d\}$) and time steps of size τ , viz.

$$\mathbf{x}_n = \begin{pmatrix} h_1 n_1 \\ \vdots \\ h_d n_d \end{pmatrix} \quad \text{with } n_i \in \mathbb{Z}, \quad (21a)$$

$$t^k = \tau k \quad \text{with } k \in \mathbb{Z}. \quad (21b)$$

The quantity \mathbf{h} will refer to a d -dimensional vector with components h_i . The discretized two-component wave function will be denoted by

$$\Psi(\mathbf{x}_n, t^k) = \begin{pmatrix} \Psi_1(\mathbf{x}_n, t^k) \\ \Psi_2(\mathbf{x}_n, t^k) \end{pmatrix} = \begin{pmatrix} \Psi_{1,n}^k \\ \Psi_{2,n}^k \end{pmatrix} = \Psi_n^k \quad (22)$$

and Ψ^k identifies a vector with components Ψ_n^k for fixed k . The discrete version of the pseudo norm (9) reads

$$\|\Psi^k\|_{\sigma_3, \mathbf{h}}^2 = \prod_{i=1}^d h_i \sum_n \Psi_n^{k*} \sigma_3 \Psi_n^k. \quad (23)$$

For the stability analysis we will also need the proper norm

$$\|\Psi^k\|_{\mathbf{h}}^2 = \prod_{i=1}^d h_i \sum_n \Psi_n^{k*} \Psi_n^k. \quad (24)$$

First and second order derivatives in (20) are approximated by finite differences. We will utilize the second order approximations $\nabla_{2,h} f(x)$ and $\nabla_{2,h}^2 f(x)$

$$\frac{\partial f(x)}{\partial x} = \nabla_{2,h} f(x) + O(h^2) = \frac{-f(x-h) + f(x+h)}{2h} + O(h^2) \quad (25a)$$

$$\frac{\partial^2 f(x)}{\partial x^2} = \nabla_{2,h}^2 f(x) + O(h^2) = \frac{f(x-h) - 2f(x) + f(x+h)}{h^2} + O(h^2) \quad (25b)$$

as well as the fourth order schemes $\nabla_{4,h} f(x)$ and $\nabla_{4,h}^2 f(x)$

$$\frac{\partial f(x)}{\partial x} = \nabla_{4,h} f(x) + O(h^4) = \frac{f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)}{12h} + O(h^4) \quad (26a)$$

$$\frac{\partial^2 f(x)}{\partial x^2} = \nabla_{4,h}^2 f(x) + O(h^4) = \frac{-f(x-2h) + 16f(x-h) - 30f(x) + 16f(x+h) - f(x+2h)}{12h^2} + O(h^4). \quad (26b)$$

Plugging (25) or (26) into (20) and taking into account boundary conditions yields the finite difference scheme (the discretized version of (15))

$$\Psi^{k+1} = U_{\mathbf{h},\tau} \Psi^k \quad (27)$$

with some sparse $2N \times 2N$ matrix $U_{\mathbf{h},\tau}$ that depends on the grid spacings \mathbf{h} and τ , where N denotes the total number of spatial grid points. Thus, the real space split operator method for the Klein-Gordon equation is essentially a matrix vector multiplication. A stability analysis has to examine the properties of this matrix vector multiplication as a function of \mathbf{h} and τ . Before we can proceed with a stability analysis, however, we have to give the term *numerical stability* a precise definition.

3. Strong and algebraic stability

Loosely speaking numerical stability of a finite difference scheme means that numerical errors that are caused by the discretization of a partial differential equation are bounded. There is no unique way to cast this intuitive notion into a formal mathematical statement and different mathematical concepts of stability may be found in the literature. We will consider the so-called strong stability [27, 28] and algebraic stability [28, 29]. An explicit finite difference scheme $\Psi^{k+1} = U_{h,\tau}\Psi^k$ for a partial differential equation, that is first-order in time, is called strongly stable in the stability region Λ if there is for any fixed positive time t a constant C such that

$$\|\Psi^k\|_h \leq C \|\Psi^0\|_h \quad \text{for all } (h, \tau) \in \Lambda, \quad 0 \leq k\tau \leq t. \quad (28)$$

Strong stability requires that the norm $\|\Psi^k\|_h$ is bounded independently of the grid spacings τ and h . An explicit finite difference scheme $\Psi^{k+1} = U_{h,\tau}\Psi^k$ for a first-order partial differential equation is called algebraically stable in a stability region $\tilde{\Lambda}$ if there are for any fixed positive time t two constants C and $\alpha \geq 0$ such that

$$\|\Psi^k\|_h \leq C\tau^{-\alpha} \|\Psi^0\|_h \quad \text{for all } (h, \tau) \in \tilde{\Lambda}, \quad 0 \leq k\tau \leq t. \quad (29)$$

Algebraic stability allows the norm to grow proportionally to $\tau^{-\alpha}$ and, therefore, it is not necessarily bounded in the limit $\tau \rightarrow 0$. Note that algebraic stability is a rather weak stability concept; there is no intermediate regime between algebraic stability and exponential explosion. Strong stability implies algebraic stability. For partial differential equations for scalar unknown functions strong and algebraic stability are equivalent. For systems of partial differential equations as the Klein-Gordon equation (3), however, strong stability does not follow by algebraic stability [28].

Strong and algebraic stability are closely related to convergence. A finite difference scheme is called convergent if the discretization error satisfies

$$\|\Psi(x, \tau k) - \Psi^k\|_h \rightarrow 0 \quad \text{for } h, \tau \rightarrow 0. \quad (30)$$

Under certain conditions, strong and algebraic stability imply convergence. A consistent finite difference scheme for a partial differential equation for which the initial value problem depends continuously on the initial condition and that is of first order in its time derivative is convergent if and only if it is strongly stable [27]. An explicit finite difference scheme $\Psi^{k+1} = U_{h,\tau}\Psi^k$ for a first order partial differential equation $i\hbar\partial\Psi(x, t)/\partial t = \hat{H}(t)\Psi(x, t)$ is called consistent if

$$\left\| \frac{\Psi^{k+1} - \Psi^k}{\tau} - \frac{U_{h,\tau} - 1}{\tau} \Psi^k - \left(\frac{\partial\Psi(x, t)}{\partial t} - \frac{1}{i\hbar} \hat{H}\Psi(x, t) \right) \right\|_h \rightarrow 0 \quad \text{for } h, \tau \rightarrow 0. \quad (31)$$

Note that a consistent strongly stable scheme is convergent independently of the initial condition. If a finite difference scheme $\Psi^{k+1} = U_{h,\tau}\Psi^k$ is algebraically stable and $U_{h,\tau}$ does not depend on spatial coordinates, then it is convergent provided that the Fourier transform $\tilde{\Psi}(p, 0)$ of the initial condition $\Psi(x, 0)$ decays faster than an appropriate power $|p|^{-l}$ for $|p| \rightarrow \infty$ [28]. Note that this condition applies only to homogeneous problems ($U_{h,\tau}$ is not allowed to depend on spatial coordinates.) and it is a sufficient condition for convergence but not necessary. The condition on the initial function $\Psi(x, 0)$ is satisfied by any function that is at least l -times differentiable and its l th derivative is absolutely integrable.

4. Stability conditions

There are various necessary and/or sufficient criteria [27, 28, 30] for strong or algebraic stability of finite difference schemes of the type (27). For example, one can show that a finite difference scheme of the type (27) is strongly stable in a region Λ if and only if for every time t , there exists a constant C such that powers of $U_{h,\tau}$ are bounded as

$$\|U_{h,\tau}^k\| \leq C \quad \text{for all } (h, \tau) \in \Lambda, \quad 0 \leq k\tau \leq t. \quad (32)$$

For a stability analysis in Fourier space one phrases the discrete function Ψ^k via its Fourier transform $\tilde{\Psi}^k(p)$, viz.

$$\Psi_n^k = \frac{1}{(2\pi)^{d/2} \prod_{i=1}^d h_i} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} \exp\left(i \sum_{i=1}^d n_i \xi_i\right) \tilde{\Psi}^k(\xi) d^d \xi. \quad (33)$$

Plugging the ansatz (33) into a finite difference scheme of type (27) for a partial differential equation with constant coefficients and assuming a spatial grid of infinite size individual Fourier modes decouple yielding a propagation equation

$$\tilde{\Psi}^{k+1}(\xi) = \tilde{U}_{h,\tau}(\xi) \tilde{\Psi}^k(\xi) \quad (34)$$

for each Fourier mode $\xi \in [-\pi, \pi]^d$. The equivalent to the condition (32) in Fourier space reads

$$\|\tilde{U}_{h,\tau}(\xi)^k\| \leq \tilde{C} \quad \text{for all } \xi \in [-\pi, \pi]^d, \quad (\mathbf{h}, \tau) \in \Lambda, \quad 0 \leq k\tau \leq t. \quad (35)$$

The condition (35) follows from (32) via Parseval's Theorem.

Proving the boundedness of powers of a matrix is often not easy, thus other criteria may be applied. The von-Neumann criterion requires for a one-step finite difference scheme with constant coefficients (27) that there is a constant K such that for all (\mathbf{h}, τ) in the stability region $\tilde{\Lambda}$ the eigenvalues $u_{h,\tau}(\xi)$ of $\tilde{U}_{h,\tau}(\xi)$ are bounded as

$$|u_{h,\tau}(\xi)| \leq 1 + K\tau. \quad (36)$$

The von-Neumann stability criterion provides a sufficient condition for algebraic stability [28]. Because strong stability implies algebraic stability, the von-Neumann stability criterion is a necessary criterion for strong stability but in general not sufficient. In the stability analysis of Sec. 5 we will use the slightly stronger criterion $|u_{h,\tau}(\xi)| \leq 1$.

5. Von-Neumann stability analysis for homogeneous potentials

In this section we are going to perform a von-Neumann stability analysis for the real space split operator method for the Klein-Gordon equation with homogeneous potentials

$$\phi(\mathbf{x}, t) = \phi_0 \quad A(\mathbf{x}, t) = A_0. \quad (37)$$

Transforming the matrix (20) with finite differences of second order (25) or fourth order (26) into Fourier space the finite difference operators in (20) have to be replaced by

$$\nabla_{3,h} f(\mathbf{x}) \rightarrow \tilde{\nabla}_{3,h} f(\xi) = -i \begin{pmatrix} \frac{\sin(\xi_1)}{h_1} \\ \vdots \\ \frac{\sin(\xi_d)}{h_d} \end{pmatrix} f(\xi) \quad (38a)$$

$$\nabla_{3,h}^2 f(\mathbf{x}) \rightarrow \tilde{\nabla}_{3,h}^2 f(\xi) = - \sum_{i=1}^d \frac{2 - 2 \cos(\xi_i)}{h_i^2} f(\xi) \quad (38b)$$

or

$$\nabla_{5,h} f(\mathbf{x}) \rightarrow \tilde{\nabla}_{5,h} f(\xi) = -i \begin{pmatrix} \frac{8 \sin(\xi_1) - \sin(2\xi_1)}{6h_1} \\ \vdots \\ \frac{8 \sin(\xi_d) - \sin(2\xi_d)}{6h_d} \end{pmatrix} f(\xi) \quad (39a)$$

$$\nabla_{5,h}^2 f(\mathbf{x}) \rightarrow \tilde{\nabla}_{5,h}^2 f(\xi) = - \sum_{i=1}^d \frac{15 - 16 \cos(\xi_i) + \cos(2\xi_i)}{6h_i^2} f_i(\xi), \quad (39b)$$

respectively. With (38) and (39) the Fourier space propagation matrix becomes for homogeneous potentials

$$\tilde{U}_{h,\tau}(\xi) = \begin{pmatrix} e^{-imc^2\tau/\hbar} \left(1 + \left(\frac{i\tau\hbar}{2m} \tilde{\nabla}_{n,h}^2 + \frac{\tau q A_0}{m} \cdot \tilde{\nabla}_{n,h} - \frac{i\tau q^2 A_0^2}{2m\hbar} \right) \right) & + \left(\frac{i\tau\hbar}{2m} \tilde{\nabla}_{n,h}^2 + \frac{\tau q A_0}{m} \cdot \tilde{\nabla}_{n,h} - \frac{i\tau q^2 A_0^2}{2m\hbar} \right) \\ - \left(\frac{i\tau\hbar}{2m} \tilde{\nabla}_{n,h}^2 + \frac{\tau q A_0}{m} \cdot \tilde{\nabla}_{n,h} - \frac{i\tau q^2 A_0^2}{2m\hbar} \right) & e^{imc^2\tau/\hbar} \left(1 - \left(\frac{i\tau\hbar}{2m} \tilde{\nabla}_{n,h}^2 + \frac{\tau q A_0}{m} \cdot \tilde{\nabla}_{n,h} - \frac{i\tau q^2 A_0^2}{2m\hbar} \right) \right) \end{pmatrix} e^{-iq\phi_0\tau/\hbar}, \quad (40)$$

where $n \in \{2, 4\}$. To derive (40) we have used that for a homogeneous scalar potential the matrix $(*)$ in (20) commutes with all other matrices in (20). The moduli of the eigenvalues of (40) do not depend on the factor $e^{-iq\phi_0\tau/\hbar}$. Therefore, for a von-Neumann stability analysis we can set $\phi_0 = 0$ without loss of generality. The numerical stability does not depend on the magnitude of the scalar potential. For convenience, we introduce the real valued quantities

$$\kappa(\xi) = \sum_{i=1}^d \kappa_i(\xi_i) \quad \text{with} \quad \kappa_i(\xi_i) = \frac{\hbar}{2m} \tilde{\nabla}_{n,h_i}^2 + \frac{q A_{0,i}}{im} \tilde{\nabla}_{n,h_i} - \frac{q^2 A_{0,i}^2}{2m\hbar} \quad (41)$$

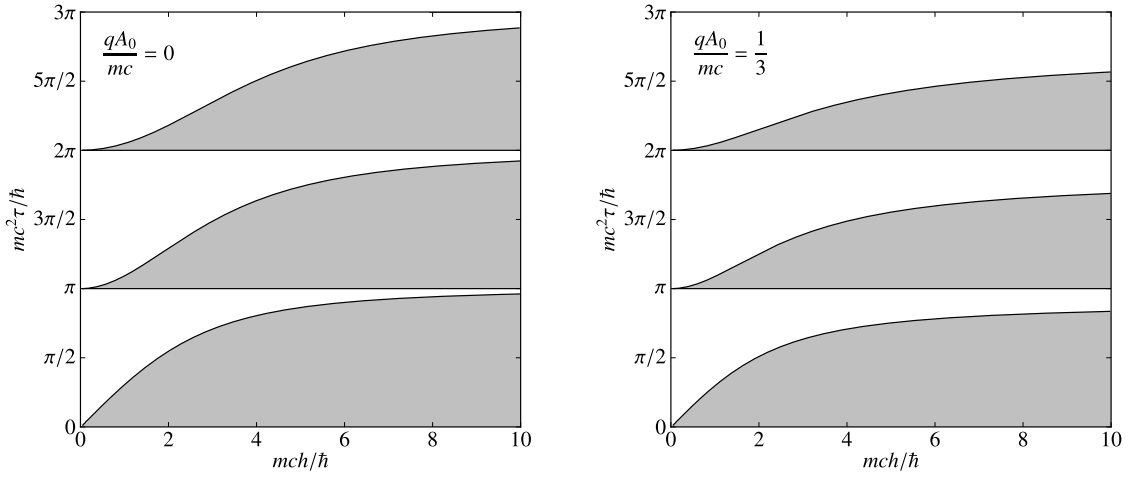


FIG. 1: Regions of algebraic stability $\tilde{\Lambda}$ (shaded in gray) for a one-dimensional finite difference scheme with three point finite differences (25) for two different values of the homogeneous vector potential A_0 as a function of the spatial grid spacing h and the temporal step width τ . The larger the vector potential the smaller the stability region.

and

$$\gamma(\xi) = \cos(mc^2\tau/\hbar) + \kappa(\xi)\tau \sin(mc^2\tau/\hbar) \quad (42)$$

such that the eigen-values of (40) are given by

$$u_{h,\tau}(\xi) = \gamma(\xi) \pm \sqrt{\gamma(\xi)^2 - 1}. \quad (43)$$

The quantity $\gamma(\xi)$ is real valued and, therefore, the von-Neumann criterion $|u_{h,\tau}(\xi)| \leq 1$ is equivalent to $\gamma(\xi)^2 \leq 1$ which must be fulfilled for every $\xi \in [-\pi, \pi]^d$. The von-Neumann criterion is fulfilled for all $\xi \in [-\pi, \pi]^d$ if it is fulfilled for all ξ^* that make $\gamma(\xi)^2$ extremal. Qualification for extremality of $\gamma(\xi)^2$ is

$$\left. \frac{\partial(\gamma(\xi)^2)}{\partial \xi_i} \right|_{\xi=\xi^*} = 2\gamma(\xi^*)\tau \sin(mc^2\tau/\hbar) \left. \frac{d\kappa_i(\xi_i)}{d\xi_i} \right|_{\xi_i=\xi_i^*} = 0 \quad \text{for all } i \in \{1, \dots, d\}. \quad (44)$$

Thus, to maximize $\gamma(\xi)^2$

$$\left. \frac{d\kappa_i(\xi_i)}{d\xi_i} \right|_{\xi_i=\xi_i^*} = 0 \quad \text{for all } i \in \{1, \dots, d\} \quad (45)$$

is required. The region $\tilde{\Lambda}$ of algebraic stability for the scheme (27) with constant potentials is finally given by

$$\tilde{\Lambda} = \left\{ (h, \tau) \in [0, \infty)^{d+1} \quad \text{with } \gamma(\xi^*)^2 \leq 1, \text{ for all } \xi^* \in [-\pi, \pi]^d \text{ that are the solutions of } \left. \frac{d\kappa_i(\xi_i)}{d\xi_i} \right|_{\xi_i=\xi_i^*} = 0 \right\}. \quad (46)$$

Figure 1 shows the region of algebraic stability $\tilde{\Lambda}$ for a one-dimensional finite difference scheme with three point finite differences (25) for two different values of the homogeneous vector potential as a function of the spatial grid spacing h and the temporal step width τ . The stability region separates into an infinite number of disconnected domains. From a practical point of view, only the stability domain that includes the point $(h, \tau) = (0, 0)$ is relevant because the temporal step width τ is not only restricted by the stability criterion (46) but also by $mc^2\tau/\hbar < \pi$. The later criterion follows from the wave-function's fast phase oscillations that are proportional to the typical energy of a wave packet which is about mc^2 . In stability domains with $mc^2\tau/\hbar > \pi$ the finite difference scheme is stable but does not give accurate numerical solutions. The shape of the stability domains depends on the modulus of the vector potential. The larger the vector potential the smaller the stability domains. The region of algebraic stability for a finite difference scheme based on five point formulas (26) looks qualitatively similar to the region for three point formulas (25) but the stability domains are slightly smaller, see Fig. 3.

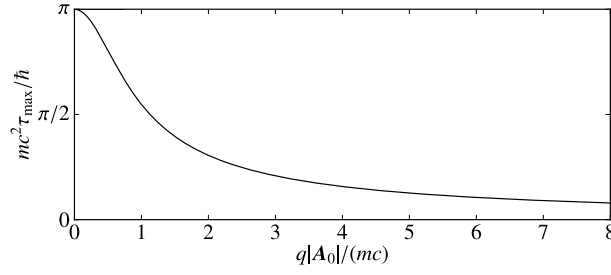


FIG. 2: Upper bound τ_{\max} on the temporal step width τ as a function of the magnitude of the vector potential A_0 .

It is instructive to analyze the region of algebraic stability $\tilde{\Lambda}$ in some limiting cases. Let us consider the case of small step widths and small vector potentials with

$$\frac{mc^2\tau}{\hbar} \ll 1, \quad \frac{mch_i}{\hbar} \ll 1, \quad \frac{q|A_{0,i}|}{mc} \ll 1 \quad \text{for all } i \in \{1, \dots, d\}$$

first. For second order finite differences (25) the condition $\gamma(\xi^*)^2 \leq 1$ yields in this limit in leading order

$$\left(1 - \frac{mc^2\tau}{\hbar} \frac{1}{2} \sum_{i=1}^d \left(\frac{mch_i}{\hbar} \right)^{-2} (2 - 2\cos(\xi_i)) \frac{mc^2\tau}{\hbar} \right)^2 \leq 1. \quad (47)$$

This expression becomes maximal for $\xi_i^* = \pm\pi$. For equal grid spacings $h_1 = \dots = h_d = h$ the condition $\gamma(\xi^*)^2 \leq 1$ simplifies to

$$\left(1 - 2d \left(\frac{c\tau}{h} \right)^2 \right)^2 \leq 1 \quad (48)$$

which is equivalent to

$$\frac{h}{\tau} > \sqrt{dc}. \quad (49)$$

A similar calculation for five point finite differences formulas (26) yields the condition

$$\frac{\sqrt{3}h}{2\tau} > \sqrt{dc}. \quad (50)$$

The other limit we want to consider is the limit of large spatial step sizes with

$$\frac{mch_i}{\hbar} \gg 1.$$

In this limit the condition $\gamma(\xi^*)^2 \leq 1$ yields for second order finite differences (25) as well as for fourth order finite differences (26) the inequality

$$\left(\cos \frac{mc^2\tau}{\hbar} - \frac{1}{2} \frac{mc^2\tau}{\hbar} \left(\frac{qA_0}{mc} \right)^2 \sin \frac{mc^2\tau}{\hbar} \right)^2 \leq 1 \quad (51)$$

which no longer depends on ξ^* . The larger the spatial steps the larger the allowed temporal step width. Thus (51) implies an upper bound on the temporal step width which we denote by τ_{\max} . Figure 2 shows τ_{\max} as a function of the magnitude of the vector potential A_0 . For a vanishing vector potential we have $mc^2\tau_{\max}/\hbar = \pi$ and $mc^2\tau_{\max}/\hbar < \pi$ otherwise.

6. Numerical results

A von-Neumann stability analysis does not account for boundary conditions, it implicitly assumes an infinite grid. Furthermore, the von-Neumann stability analysis is not applicable to systems with spatially dependent potentials. Thus, we are going to compare our analytical results of Sec. 5 with the stability of actual numerical simulations that work on finite grids and implement the boundary condition that the wave function vanishes at border. We will determine the numerical stability for systems with spatially dependent potentials as a function of the size of the grid spacings and compare the results with the predictions of our von-Neumann stability analysis for homogeneous potentials. In all our numerical simulations atomic units (a.u.) with $\hbar = 1$ a.u., $q = e = 1$ a.u., $m = 1$ a.u., and $c \approx 137.036$ a.u. will be applied.

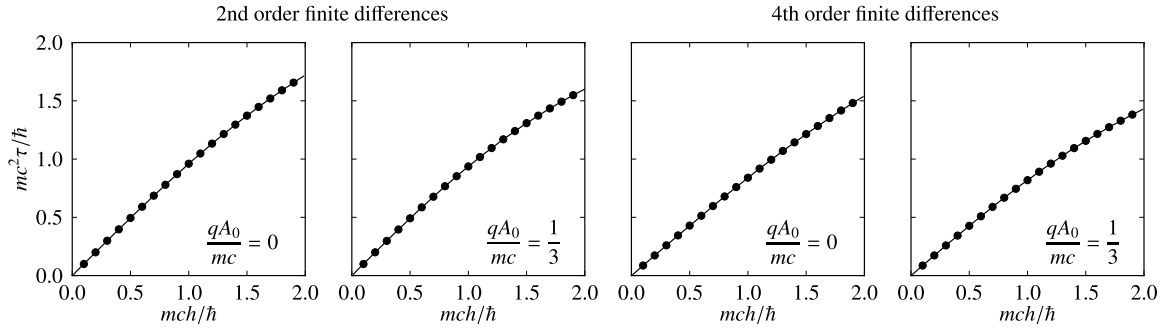


FIG. 3: Comparison of the critical lines as predicted by (46) (solid lines) with the points of transition from stability to instability as they have been observed in actual numerical simulations (filled circles) of one-dimensional wave packets using finite differences of second order (25) and of fourth order (26), respectively.

6.1. Systems with homogeneous potentials

In order to check the condition (46) we determined the region of stability also numerically by propagating a one-dimensional wave packet in homogeneous potentials using different grid spacings h and τ . The initial wave packet was given by a Gaussian superposition of positive energy free particle eigen-states with momentum p

$$\Psi(x, 0) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \frac{1}{2(1 + p^2/(mc)^2)^{1/4}} \left(\frac{1 + \sqrt{1 + p^2/(mc)^2}}{1 - \sqrt{1 + p^2/(mc)^2}} \right) \frac{1}{(2\pi\Delta^2)^{1/4}} \exp\left(-\frac{(p - \bar{p})^2}{4\Delta^2} + i\frac{xp}{\hbar}\right) dp. \quad (52)$$

The initial wave packet has mean momentum \bar{p} and momentum width Δ . For our tests we chose $\bar{p} = 20$ a.u., $\Delta = 1$ a.u. and a computational grid that ranges from $x_{\text{left}} = -3$ a.u. to $x_{\text{right}} = 5$ a.u. The wave packet was propagated from time $t_{\text{init}} = 0$ a.u. to $t_{\text{end}} = 1/20$ a.u. For a free wave packet not only the pseudo norm (9) is conserved but also the Euclidean norm (10). Thus, numerical stability may be checked by determining if the discrete norm (24) grows exponentially or not as a function of the grid spacings h and τ . Figure 3 presents our results for two different vector potentials and finite difference formulas of second order (25) and of fourth order (26), respectively. We observe an excellent correspondence between the von-Neumann stability analysis result (46) and our numerical findings.

6.2. Systems with spatially dependent potentials

We considered so far systems with homogeneous potentials only. In numerical calculations, however, one typically wants to simulate systems with spatially dependent potentials to which the technique of the von-Neumann stability analysis is not applicable. It is possible to show that the results of von-Neumann stability analysis for systems with homogeneous potentials can generally not be extended to inhomogeneous systems. In particular, one can devise finite difference schemes for partial differential equations that are unstable although the von-Neumann condition (36) is satisfied locally everywhere [28].

Assuming that the stability properties of the real space split operator method are well behaved one expects that for systems with potentials that vary on length scales that are large compared to the size of the wave packet the stability region is given in close approximation by (46). If the stability is actually affected by the potentials' spatial dependence then it is expected to have a larger impact, if the potentials vary on the length scale that is given by the wave-function's width. In order to test how a spatially dependent vector potential changes the stability properties of the real space split operator method we simulated scattering of a free wave packet on a strong laser pulse having a very short wave length.

We start with a two-dimensional Gaussian wave packet

$$\Psi(\mathbf{x}, 0) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{2(1 + \mathbf{p}^2/(mc)^2)^{1/4}} \left(\frac{1 + \sqrt{1 + \mathbf{p}^2/(mc)^2}}{1 - \sqrt{1 + \mathbf{p}^2/(mc)^2}} \right) \frac{1}{(2\pi\Delta^2)^{1/2}} \exp\left(-\frac{\mathbf{p}^2}{4\Delta^2} + i\frac{\mathbf{x}\mathbf{p}}{\hbar}\right) d\mathbf{p}. \quad (53)$$

The wave packet evolves in a laser pulse of wave length λ with the electromagnetic fields

$$\mathbf{E}(\mathbf{x}, t) = \mathbf{E}_0 \sin(\mathbf{k} \cdot \mathbf{x} - \omega t) f_{j,l}(\mathbf{k} \cdot \mathbf{x} - \omega t), \quad (54a)$$

$$\mathbf{B}(\mathbf{x}, t) = \frac{\mathbf{E}_0}{c} \sin(\mathbf{k} \cdot \mathbf{x} - \omega t) f_{j,l}(\mathbf{k} \cdot \mathbf{x} - \omega t) \quad (54b)$$

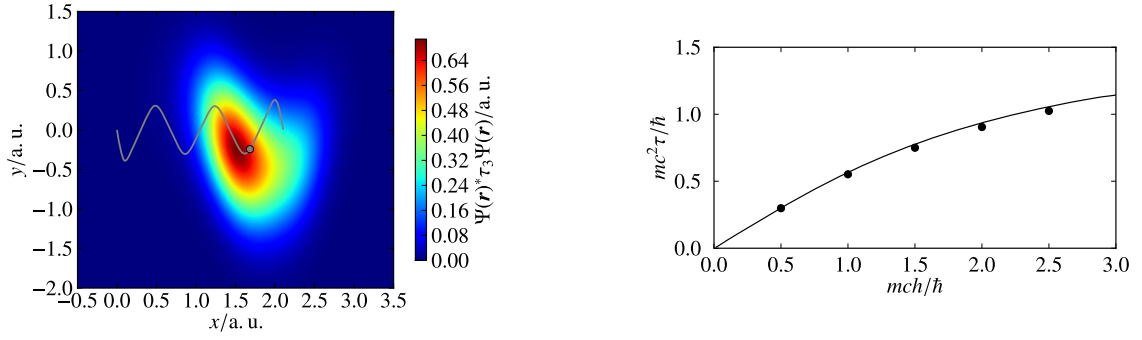


FIG. 4: Left panel: Motion of a wave packet in a ultra strong laser field. Plot shows the center of mass motion (gray line) and a snapshot of the density (7) with the corresponding center of mass (gray circle). Right panel: Stability line for the system in the left panel using fourth order finite differences. Dots indicate critical points as determined numerically, the solid line is given by (46) using the vector-potential's maximal value.

with $|\mathbf{k}| = 2\pi/\lambda = \omega/c$ and $\mathbf{E}_0 \perp \mathbf{k}$ and an envelope function $f_{j,l}(\eta)$ of total j half cycles including a linear turn-on ramp and a linear turn-off ramp of l half cycles and a constant plateau in between, viz.

$$f_{j,l}(\eta) = \begin{cases} (\eta + j\pi)/(l\pi) & \text{if } -j \leq \eta/\pi \leq -j + l, \\ 1 & \text{if } -j + l \leq \eta/\pi \leq -l, \\ -\eta/(l\pi) & \text{if } -l \leq \eta/\pi \leq 0, \\ 0 & \text{else.} \end{cases} \quad (54c)$$

The corresponding vector potential follows from (54) via

$$\mathbf{A}(\mathbf{x}, t) = - \int_0^t \mathbf{E}(\mathbf{x}, t') dt'. \quad (55)$$

For our simulation we chose the parameters $\Delta = 1$ a.u., $\lambda = 3$ a.u., $j = 8$, $l = 2$ and $|\mathbf{A}_0| = |\mathbf{E}_0|/\omega = mc/q$. The initial wave packet has a width of a half Bohr radius and scatters at an ultra strong laser pulse having wave length only six times larger and a peak intensity of 1.09×10^{26} W/cm². The left panel of Fig. 4 shows the center of mass motion and a snapshot of the density (7).

Determining the numerical stability by propagating the wave function using different step widths $h_1 = h_2 = h$ and τ we find that the stability region for this system with spatially dependent vector potential agrees well with (46) if in (46) the maximal value of (55) is used, see right panel of Fig. 4. Numerical instability was detected by determining if (24) grows exponentially or not. Note that for a wave packet in a laser field the norm (24) is not a conserved quantity. Our numerical findings suggest the conjecture that the real space split operator method is stable also for inhomogeneous potentials if the von-Neumann condition (36) is satisfied locally everywhere.

7. Conclusions

We analyzed the stability of a real space split operator method for the time-dependent Klein-Gordon equation and found that the method is conditionally stable. For homogeneous potentials the region of algebraic stability was determined as (46) via a von-Neumann stability analysis. Our numerical simulations support the conjecture that the condition (46) is also applicable for spatially dependent vector potentials. In the limit of small spatial grid spacings h in all spatial directions and small temporal steps τ the stability condition becomes $h/\tau > \sqrt{dc}$ for second order finite differences and $\sqrt{3}h/(2\tau) > \sqrt{dc}$ for fourth order finite differences, respectively. Two conditions that might be more handy for practical applications. Our results may help to circumvent numerical instabilities in the application of the real space split operator method for the Klein-Gordon equation by choosing appropriate spatial grid spacings and an appropriate temporal step width.

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